Pairing Gap and Polarisation Effects

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The phenomenological adjustment of the nuclear pairing strength is usually performed with respect to the odd-even staggering of the binding energies. We find that the results strongly depend on the way in which the ground states of the odd nuclei are computed. A thorough calculation including all time-even and time-odd polarisation effects induced by the odd nucleon produces about 30% reduced odd-even staggering as compared to the standard spherical calculations in the relativistic mean-field model. The pairing strength must be enhanced by about 20% to compensate for that effect. The enhanced strength has dramatic consequences for the predicted deformation properties of the underlying mean-field models, possibly implying that new adjustments of their parameters become necessary as well.

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Pairing is an essential ingredient of nuclear mean-field models since the early days of the single-particle shell model [1,2]. It can be motivated from a theoretical point of view by a near-singularity of the effective T matrix near the Fermi surface [3] and it manages to subsummarize a large amount of two-body correlations at the price of a moderately extended mean-field theory. From a phenomenological point of view, pairing is needed to explain, e.g., the existence of spherical non-magic nuclei and to account for the observed strong odd-even staggering of the binding energies. The purely theoretical access to pairing from nuclear many-body theory is still plagued by unresolved quantitative problems of nuclear "ab initio" calculations [4]. One thus has to recur to phenomenological information which is exploited nowadays with a high degree of systematics (for a recent and comprehensive compilation see [5]). The general strategy of these phenomenological evaluations is to relate the odd-even staggering of the binding energies to the pairing gap by taking appropriate differences, e.g., for neutrons the fourth order difference

$$\Delta_n^{(4)} = -\tfrac{1}{8}(-1)^N \big[E(N-2) - 4E(N-1) + 6E(N) \\ -4E(N+1) + E(N+2)\big] \qquad (1)$$

at fixed proton number. This access, however, has the basic problem that pairing is not the only source of odd-even staggering. Odd-even fluctuations in energy can also be produced by polarisation of the even core through the odd nucleon, which leads to odd-even jumps in deformation, spin-alignment or dynamical currents. For example, there is pronounced odd-even staggering in the energies of metal clusters which, however, can be explained exclusively by effects of spin-alignment and Jahn-Teller deformation [6]. Spin alignment can be excluded for most nuclei. The Jahn-Teller effect alone can produce sizeable odd-even effects in deformed nuclei as was worked out in a recent paper [7], but its influence is diminished for semi-magic nuclei if pairing is switched on because this restores spherical symmetry over the whole isotopic or isotonic chain. Nonetheless, there remains a polarisation of the core through the field of the odd nucleon, which may deliver substantial contributions to the odd-even staggering and thus should be taken into account when adjusting pairing strengths to the phenomenological pairing gap (1). The question is how large these polarisation effects are in practice. There is, first, the static deformation-polarisation which is induced by the finite multipole moment of the odd nucleon's density. In addition the odd nucleon breaks the intrinsic time-reversal invariance because it carries a nonzero spin and a current contribution. These time-odd components can induce a sizeable time-odd response in terms of spin and current polarisation in the even-even core [8]. In the following we call that a dynamical polarisation to distinguish it from the mere deformation effects. It is the aim of this letter to investigate the effect of such polarisation effects on the odd-even staggering and thus on the adjustment of the pairing gap (1).

The investigation requires a mean-field model which provides reliable response properties in all channels, including unnatural parity states and spin polarisation. The relativistic mean-field (RMF) model includes a "natural" description of spin properties [8–10] and is a reliable starting point for our present investigation of dynamical polarisation. A similar investigation on the grounds of the non-relativistic Skyrme-Hartree-Fock model was performed recently [11]. We employ the RMF with the parametrization PL-40 [12] similar as in a previous systematic investigation of odd nuclei near magic shells [8]. The details of the model, the strategy to define the blocking in odd nuclei, and the numerical handling can be found there. We perform axially symmetric deformed calculations including time-odd currents to take into ac-

approach	V_n (MeV fm^3)	$\Delta_n^{(4)}$ (MeV)
exp.		1.2587
spherical	−346.0	1.2493
deformed	−346.0	1.1600
dyn. polarisation	−346.0	0.8104
	−412.4	1.2588

TABLE I. Neutron gaps $\Delta_n^{(4)}$ in ^{126}Sn for the various levels of approximation. In case of dynamical polarisation the gaps are shown for the original as well as for the refitted pairing strength V_n (last line).

count the broken time-reversal symmetry and its related polarisation effects. Pairing is described at the BCS level using matrix elements computed from a zero-range pairing force $V_q\,\delta(\mathbf{r}_1 - \mathbf{r}_2)$ with $q \in \{p, n\}$ acting in a pairing space which is limited by a soft cut-off of Woods-Saxon shape in energy [13,14] with the cut-off adjusted dynamically to include $N_q + 1.65\,N_q^{2/3}$ nucleon states [15]. The pairing strengths are fitted to the experimental gaps within several semi-magic isotope and isotone chains in connection with the actual mean-field force. The odd nuclei needed for this approach are calculated in a spherical approximation. For PL-40, which is used in this study, we find $V_p = -348$ MeV fm^3 and $V_n = -346$ MeV fm^3. These values correspond to a standard determination of pairing strengths without polarisation effects. We take them as a base point for comparison with the more elaborate adjustments to be discussed in the following.

As a test case we consider the neutron gaps in the chain of Sn isotopes. The magic proton number in Sn allows to concentrate on the neutron gaps and it renders all even isotopes spherical, which confines the deformation effects exclusively to the odd isotopes.

Figure 1 shows the results for the neutron gap (1) at various levels of mean-field calculations: spherically, deformed but time-even, and deformed with dynamical polarisation (i.e., including time-odd currents). As mentioned above, the spherical results had been fitted to agree with the experimental gaps in the average, which has been achieved more or less nicely. Allowing for deformation (yet without dynamical polarisation) indeed changes the gaps at several isotopes. For the heavier nuclei, however, to which pairing is usually fitted, the resulting reduction of the gap is sufficiently small to neglect them at the level of quality with which pairing can be adjusted anyway. This can be deduced from the small changes from “spherical” to “deformed” seen in fig. 1. The effect is much larger when allowing for dynamical polarisation. The gaps shrink in average by about 30%. The example here shows that dynamical polarisation can have a large effect on the odd-even staggering which, in turn, puts a warning signs on a phenomenological adjustment of pairing properties on the the basis of energy differences. One should, in fact, adjust the gaps (1) anew while using fully polarised calculations.

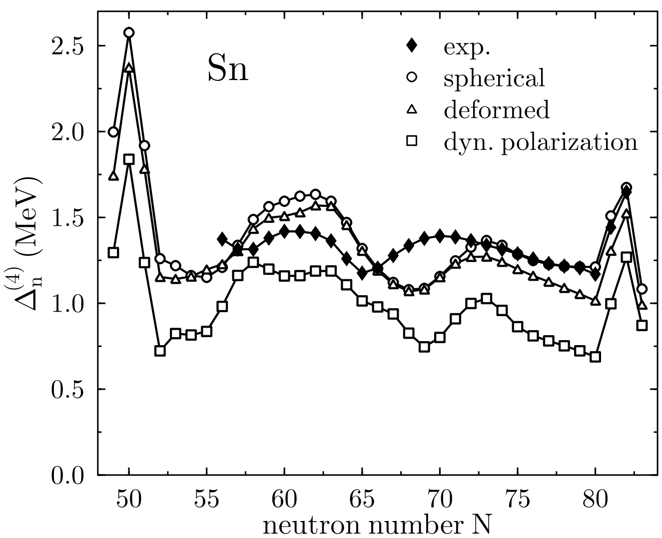

FIG. 1. Fourth-difference neutron gaps (1) for Sn isotopes ($Z = 50$) computed with the RMF parametrization PL-40 in different approaches. Spheres stand for purely spherical calculations without time-odd currents, triangles for deformed calculations without time-odd currents, and squares for unrestricted deformed calculations including time-odd currents. Experimental gaps are given as full rhombi for comparison (the masses were taken from [16]).

In order to check that this reduction of the gap is not a particular feature of PL-40, we have performed similar calculations for the parametrization NL3 [17] which was adjusted with different bias. we find for the case of ^{126}Sn the sequence 1.32 MeV for the gap from spherical calculations, over 1.30 MeV for the gap from deformed and time-even calculations down to 0.93 MeV for the case with full dynamical polarisation. That is very much the same reduction as explored for PL-40, see Table I. we thus are confident that the effect is of generic nature, at least for the RMF.

We now want to exemplify the consequences of such a modified pairing strength for the present test case. To that end, we have performed a readjustment of the pairing strength taking properly into account all polarisation effects. In order to cope with the rather large expense of the full-fledged calculations of odd nuclei, we have decided to concentrate on the neutron pairing strength and to refit that with respect to one nucleus, namely ^{126}Sn. We find that the readjustment (including time-odd currents) increases the required pairing-strength parameter by as much as 19%. Proton pairing will be needed in two applications later on. We find that the same enhancement factor of 19% reproduces gaps in heavy nuclei very well. For that we assume the same upscaling factor as was found for neutron pairing. This minimal fitting strategy is sufficient for the present purposes of an exploratory study. The results for the case of neutron pairing in ^{126}Sn are summarised in table I. One sees that the dynamical polarisation reduces the gap by 35% in this case and a counteracting readjustment increases

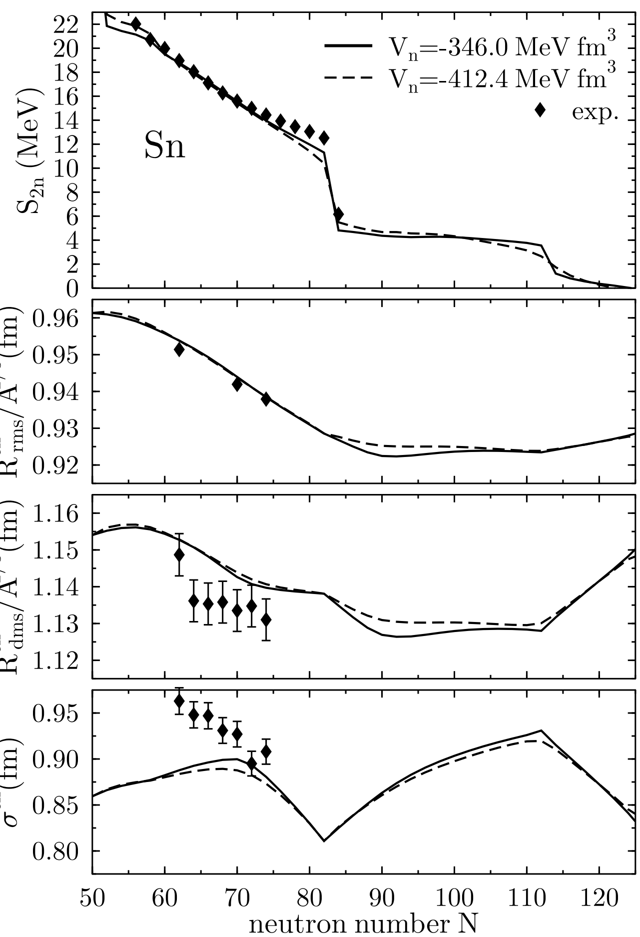

FIG. 2. Ground state observables in Sn isotopes drawn as functions of the neutron number N. Upper panel: two-neutron separation energies $S_{2n} = E(N-2) - E(N)$; second from above: rms radii of the charge distribution, $R^{\rm ch}_{\rm rms}$; third panel: diffraction radii $R^{\rm ch}_{\rm dms}$; lowest panel: surface thickness σ. The error bars represent the average precision of the mean field model to reproduce these quantities (the actual experimental errors would be much smaller). Two cases are compared: a calculation with the spherically fitted pairing strength (full lines) and with the refitted strength (dashed lines).

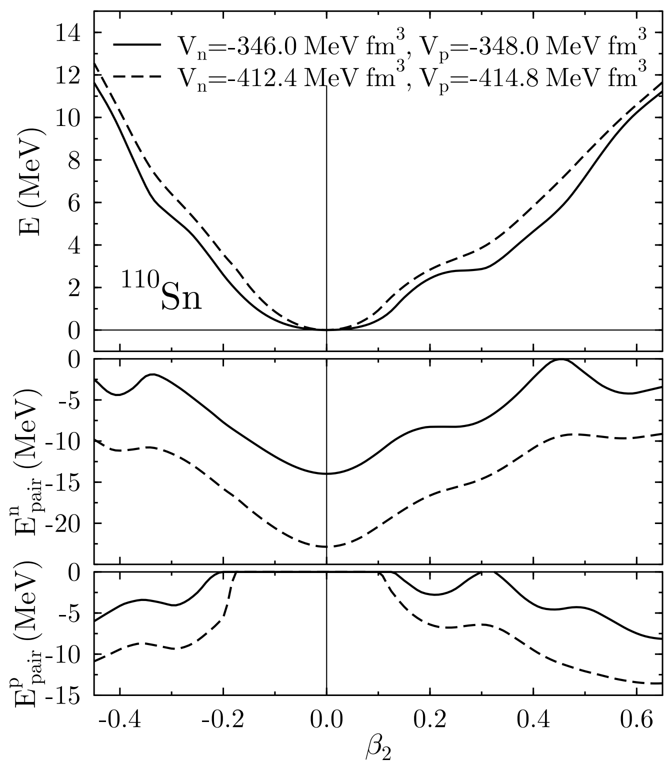

FIG. 3. Quadrupole deformation properties for ^{110}Sm drawn versus the dimensionless quadrupole deformation $\beta_2 = \left[4\pi/(3AR^2)\right]\langle r^2 Y_{20}\rangle$ with $R = 1.2$ fm $A^{1/3}$. The full line shows the result obtained with standard pairing (fitted to spherically calculated nuclei only) and the dashed line those for the enhanced pairing strength (fitted including polarisation effects). Upper: Deformation energy, i.e. total energy rescaled to zero at the spherical minimum. Middle: Neutron pairing energy. Lower: Proton pairing energy.

the pairing-strength parameter by 19%. It remains to check the consequences for other observables.

A summary of ground-state properties is shown in fig. 2. The binding energies are displayed in terms of the two-neutron separation energies $S_{2n}(N,Z) = E(N-2,Z) - E(N,Z)$ because this amplifies possible effects. The overall size and trend is not much affected by the change of the pairing strength. There is, however, a systematic modification near the shell closures. Consider, e.g., the magic $N = 82$. The larger, refitted pairing strength produces a smaller S_{2n} before this shell and a larger S_{2n} right after it. The jump of the two-neutron separation energies at a magic shell serves as an empirical measure of the “magicity”, called the two-neutron shell gap. And we see that this shell gap is reduced by as much as 25% when employing the refitted pairing strength. The binding energies as such are slightly enhanced by at most 0.25% in the mid-shell region due to the stronger pairing. This change can be, and needs to be, corrected by a slight readjustment of the RMF parametrization.

Fig. 2 also shows the bulk properties of the nuclear charge distribution, i.e., root-mean-square radii [18], diffraction radii, and surface thicknesses [19]. There are small effects visible but they remain far below the precision of the force to describe these observables (indicated by the error bars). Density and formfactor are thus rather robust against this change in pairing strength.

The situation may be different for deformation properties because these are known to result from an interplay between shell structure and pairing. As an example, in fig. 3 we show the quadrupole deformation energy for ^{110}Sm, the softest member of the Sn isotope chain. The results confirm the rule-of-thumb that stronger pairing acts more to restore the spherical shape. The refitted, enhanced pairing strength clearly produces a stiffer deformation energy curve and suppresses more efficiently

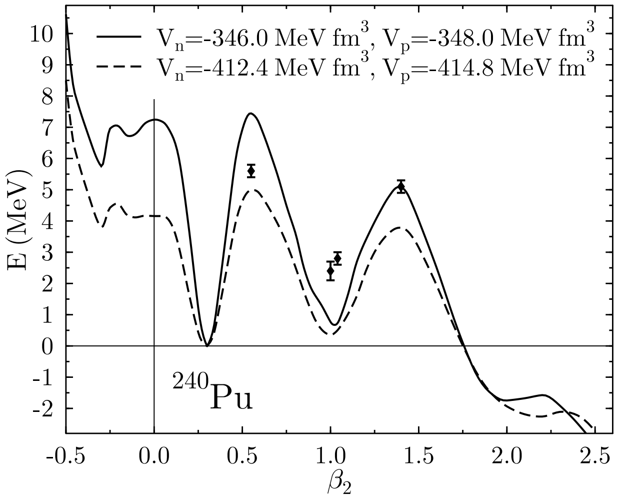

FIG. 4. Deformation energy curve (defined as in as fig. 3) for ^{240}Pu. The points with error bars show the experimental minima and barriers [20,21].

the deformed side minima which are visible in case of the standard pairing strengths. It is worthwhile to estimate the consequences for the low-lying 2^+ state. The curvature at $\beta_2 = 0$ is enhanced by about 130%. The cranking mass is proportional to the inverse quasiparticle energies which are enhanced by about 35% for the refitted pairing strengths. The mass is thus reduced by 25% and the energy of the low-lying 2^+ state is then altogether increased by about 60% for the refitted pairing strengths. This little estimate demonstrates that an appropriate determination of the pairing strength is crucial for these low-lying collective modes.

The two lower plots of fig. 3 show the proton and neutron pairing energies versus deformation. The larger refitted strength yields, of course, much larger pairing energies (absolute values), but it does also produce a larger diffuseness of occupation numbers near the Fermi surface which, in turn, degrades the mean-field binding leaving altogether the net effect of a stiffer deformation energy curve as seen in the upper panel of the figure. The example does also show the breakdown of pairing towards the proton shell closure at spherical shape, and it shows that the breakdown comes, of course, a bit later for the stronger pairing. This feature, however, should not be overstressed because the breakdown is anyway an artefact of the mere BCS treatment. A more correct approach would be to use particle number projection. But the main effect on the deformation energy curve will not be changed by that.

Other important observables in nuclear physics are fission barriers and it is worth looking at the effect when the pairing strengths are changed. Fig. 4 shows the energy curve for asymmetric fission of ^{240}Pu. For this heavy nucleus, we see even more dramatic changes. The (deformed) minima are softened such that the curvature is reduced by a factor of two. At first glance, one may be surprised to see here a softening whereas the higher pairing strength caused a stronger curvature in case of ^{110}Sn. It is to be noted that the minima in these two cases have different origins. For ^{110}Sn, the high level density at spherical shape inhibits, in principle, a spherical minimum and sphericity is only restored by the action of pairing. Consequently, stronger pairing makes the spherical shape even more pronounced. For ^{240}Pu, on the other hand, the deformed minimum is caused by a low level density at this place and pairing can only counteract this preference, thus delivering a softening of the minimum. There may be, nonetheless, only a small effect on the energy of the vibrational states in the deformed minima because the quasiparticle energies (and with them the Inglis mass) are enhanced also by about a factor of two. On the other hand there is a strong effect on fission properties because the barriers are lowered by 1–2 MeV. The change of the barriers moves them away from the experimental points for this particular mean-field parametrization (note that the inner barrier would be further lowered when allowing for triaxial shapes). This means that the selection of the appropriate parametrization for fission [22] needs to be reconsidered in connection with the new pairing strength.

Altogether, we find that dynamical polarisation effects can have a strong influence on the pairing gap as deduced from even-odd staggering of binding energies. In the present test case, one needs to enhance the underlying pairing strengths by about 20% to compensate for that effect. This change in pairing strengths has only a small effect on the ground state properties of even-even nuclei like binding energies and radii. But more elaborate quantities like the jump of the two-particle separation energies at magic shells can react sensitively. Even more dramatic changes are seen for deformation properties. Vibrations around spherical shapes become more rigid and fission barriers are significantly lowered. These findings are disquieting and call for further critical inspection with different test cases and other mean-field theories. There is, for example, one possible flaw in the RMF. It is an effective Hartree theory. Thus the polarisation energy in the odd nucleus contains a contribution from the self-interaction of the odd nucleon and a self-interaction corrected theory may produce different results. The situation is different in the non-relativistic Skyrme–Hartree–Fock model which can be considered as a true Hartree-Fock variational theory and which thus is free from the self-interaction effect. Research in this direction is underway.

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